



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 103003

TO: Mojdeh Bahar
Location: CM1/3E11&2B19
Art Unit: 1617
Friday, September 05, 2003

Case Serial Number: 09/544984

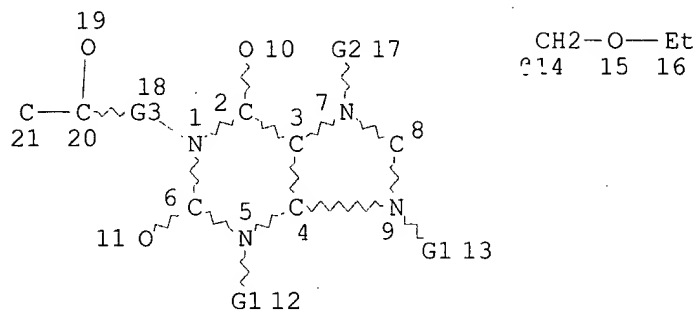
From: David Schreiber
Location: Biotech-Chem Library
CM1-6A03
Phone: 308-4292

david.schreiber@uspto.gov

Search Notes

=> d que 123

L8 STR



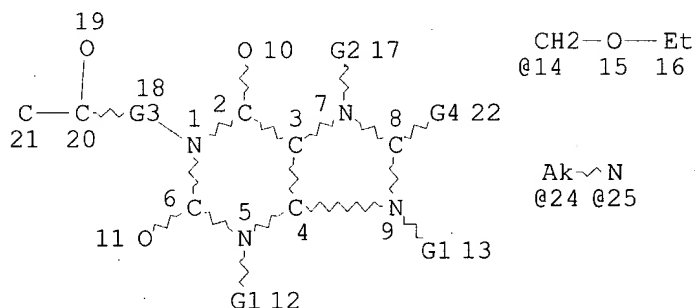
L8
Main structure
without limitations
for Z in claims

VAR G1=H/CH3
VAR G2=H/CH3/14
REP G3=(3-7) C
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 10
CONNECT IS E1 RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE
L10 53 SEA FILE=REGISTRY SSS FUL L8
L20 STR

← structures found for L8



L20
Substructure with
limitations for Z

VAR G1=H/CH3
VAR G2=H/CH3/14
REP G3=(3-7) C
VAR G4=N/24/25
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 10
CONNECT IS E1 RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L22
L2315 SEA FILE=REGISTRY SUB=L10 SSS FUL L20
3 SEA FILE=HCAPLUS L22

← structures found for L20
← 3 references having these structures in L22

=> d ibib abs hitstr 123 1-3

L23 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:575761 HCAPLUS

DOCUMENT NUMBER: 137:140535

TITLE: Preparation of tricyclic fused xanthines for treatment of disorders affected by cytokine intracellular signaling.

INVENTOR(S): Gong, Baoqing; Klein, J. Peter; Coon, Michael

PATENT ASSIGNEE(S): Cell Therapeutics, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 32 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002103211	A1	20020801	US 2000-725016	20001129
US 6586429	B2	20030701		
WO 2002068421	A2	20020906	WO 2001-US43048	20011109
WO 2002068421	A3	20030731		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

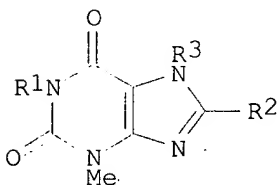
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003162801 A1 20030828 US 2003-349935 20030124

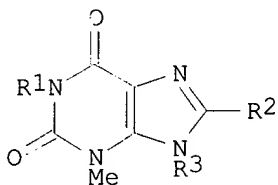
PRIORITY APPLN. INFO.: US 2000-725016 A 20001129

OTHER SOURCE(S): MARPAT 137:140535

GI.



I



II

AB Title compds. [I, II; R1 = H, (substituted) alkyl, alkenyl, alkynyl, hydroxyalkyl, cyanoalkyl, alkoxy, alkoxyalkyl; R2R3 = atoms to form a (substituted) heterocyclyl], were prepd. Thus, to (R)-7,8-dihydro-3-(5-hydroxyhexyl)-1-methyl-1H-imidazo[2,1-f]purine-2,4(3H,6H)-dione (CT-13430) and imidazole in DMF was added tert-butyldimethylsilyl chloride. Stirring

for 16 h gave 100% (R)-7,8-dihydro-1-methyl-3-(5-tert-butylidimethylsilyloxyhexyl)-1H-imidazo[2,1-f]purine-2,4(3H,6H)-dione, which with p-dimethylaminopyridine in CH₂Cl₂ was treated with Ac₂O. Stirring at room temp. for 2 h followed by chromatog. gave 67% (R)-8-acetyl-7,8-dihydro-1-methyl-3-(5-tert-butylidimethylsilyloxyhexyl)-1H-imidazo[2,1-f]purine-2,4(3H,6H)-dione. The latter in MeOH was treated with HCl in Et₂O. After stirring at room temp. for 30 min, the reaction mixt. was treated with Et₃N. Conc. under reduced pressure gave a white solid which was treated with H₂O and stirred for 1 h. The solid was filtered, washed with H₂O, and dried under vacuum to provide (R)-8-acetyl-7,8-dihydro-3-(5-hydroxyhexyl)-1-methyl-1H-imidazo[2,1-f]purine-2,4(3H,6H)-dione (CT-30260). CT-30260 suppressed Th1 differentiation by blocking IL-12 signalling with IC₅₀ = 9 .mu.M.

IT 444602-76-0P 444602-77-1P 444602-78-2P

444602-84-0P

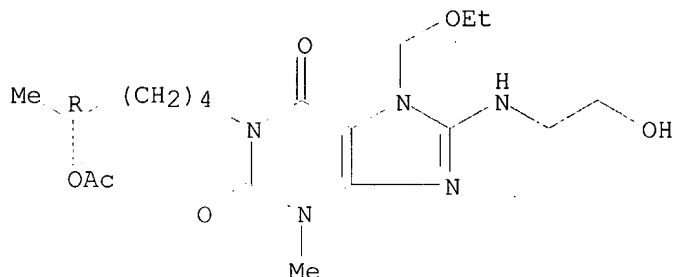
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of tricyclic fused xanthines for treatment of disorders affected by cytokine intracellular signaling)

RN 444602-76-0 HCAPLUS

CN 1H-Purine-2,6-dione, 1-[(5R)-5-(acetyloxy)hexyl]-7-(ethoxymethyl)-3,7-dihydro-8-[(2-hydroxyethyl)amino]-3-methyl- (9CI) (CA INDEX NAME)

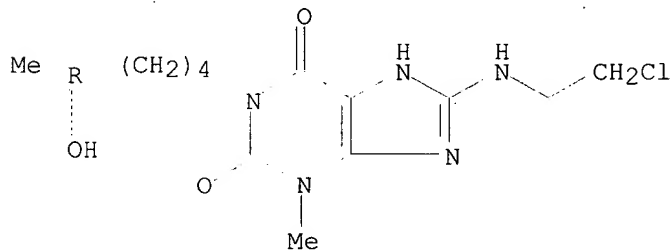
Absolute stereochemistry.



RN 444602-77-1 HCAPLUS

CN 1H-Purine-2,6-dione, 8-[(2-chloroethyl)amino]-3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl- (9CI) (CA INDEX NAME)

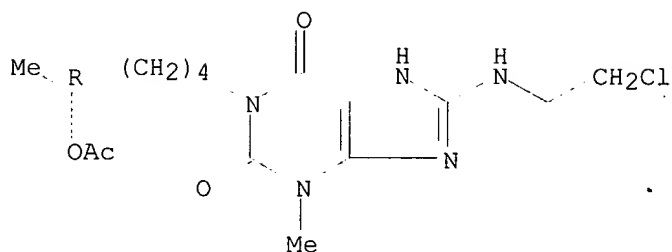
Absolute stereochemistry.



RN 444602-78-2 HCAPLUS

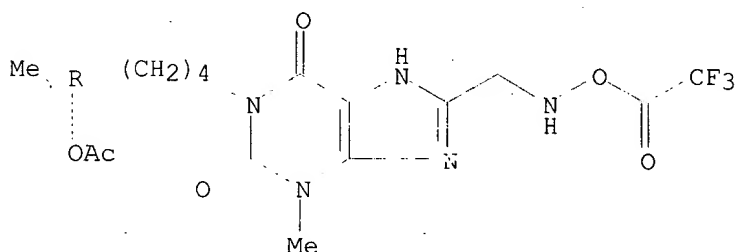
CN 1H-Purine-2,6-dione, 1-[(5R)-5-(acetyloxy)hexyl]-8-[(2-chloroethyl)amino]-3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 444602-84-0 HCAPLUS
 CN 1H-Purine-2,6-dione, 1-[(5R)-5-(acetyloxy)hexyl]-3,7-dihydro-3-methyl-8-
 [[[(trifluoroacetyl)oxy]amino]methyl]- (9CI) (CA INDEX NAME)

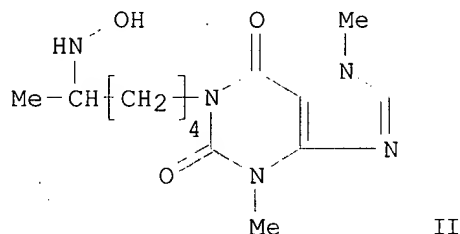
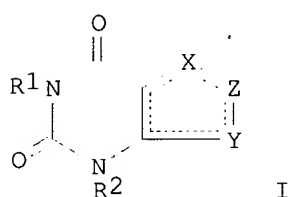
Absolute stereochemistry.



L23 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:172492 HCAPLUS
 DOCUMENT NUMBER: 136:232165
 TITLE: Preparation of xanthine derivatives and analogs as
 cell signaling inhibitors
 INVENTOR(S): Klein, J. Peter; Klaus, Stephen J.; Kumar, Anil M.;
 Gong, Baoqing
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 143 pp., Cont.-in-part of U. S.
 Ser. No. 8,020, abandoned.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 8
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002028823	A1	20020307	US 1999-233556	19990409
US 6469017	E1	20021022	US 1996-8020	19980116
WO 2000061583	A1	20001019	WO 2000-US9139	20000407
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,				
CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,				
IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,				
MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,				
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,				
AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,				
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,				

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 EP 1171442 A1 2C020116 EP 2000-921774 20000407
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO
 JP 2002541258 T2 20021203 JP 2000-610854 20000407
 PRIORITY APPLN. INFO.: US 1998-8020 B2 19980116
 US 1995-483871 A2 19950607
 US 1995-486264 A2 19950607
 US 1999-288556 A2 19990409
 WO 2000-US9139 W 20000407
 OTHER SOURCE(S): MARPAT 136:232165
 GI



AB Therapeutic compds. I [R1 = H, Me, (un)substituted C5-9-alkyl, C5-9-alkenyl, C5-9-alkynyl, C3-8-hydroxyalkyl, C3-8-alkoxy, C5-9-alkoxyalkyl; R2, R3 = H, halo, oxo, (un)substituted C1-20-alkyl, C1-20-hydroxyalkyl, C(1-20)thioalkyl, C1-20-alkylamino, C1-20-alkylaminoalkyl, C1-20-aminoalkyl, C1-20-aminoalkoxyalkenyl, C1-20-aminoalkoxyalkynyl, C1-20-diaminoalkyl, C1-20-triaminoalkyl, C1-20-tetraaminoalkyl, C5-15-aminotrialkoxyamino, C1-20-alkylamido, C1-20-alkylamidoalkyl, C1-20-amidoalkyl, C1-20-acetamidoalkyl, C1-20-alkenyl, C1-20-alkynyl, C3-8-alkoxyl, C1-11-alkoxyalkyl, and C1-20-dialkoxyalkyl; with the proviso that R1 .noteq. .omega.-1 secondary alc. substituted C5-8-alkyl; X, Y = NR3, R3 = C1-3-alkyl; Z = CR3, R3 = C1-3-alkyl; dashed lines are single or double bonds] pharmaceutically acceptable derivs. (e.g., resolved enantiomers, diastereomers, tautomers, salts and solvates thereof) or prodrugs thereof are described. Thus, CT 7549 (II) was prepd. via redn of 1-(5-oximinohexyl)-3,7-dimethylxanthine using sodium cyanoborohydride in methanol. These novel heterocyclic compds. I having a six membered ring structure fused to a five membered ring structure are found to be useful for the treatment and prevention of symptoms or manifestations assocd. with disorders affected by Interleukin-12 ("IL-12") intracellular signaling, such as, for example, Th1 cell-mediated disorders.

IT 301536-55-0P, CT 12440 301536-56-1P, CT 12441
 301536-57-2P, CT 12447 301536-64-1P, CT 12481
 403477-24-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

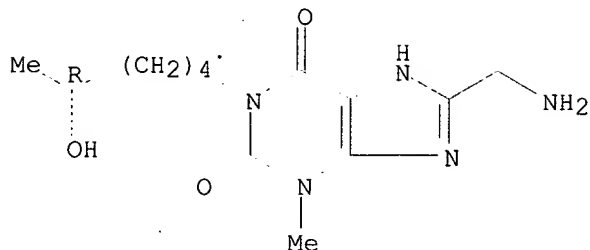
(prepn. of xanthine derivs. and analogs as cell signaling inhibitors)

RN 301536-55-0 HCAPLUS

CN 1H-Purine-2,6-dione, 8-(aminomethyl)-3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl- (9CI) (CA INDEX NAME)

Bahar 09/544,984

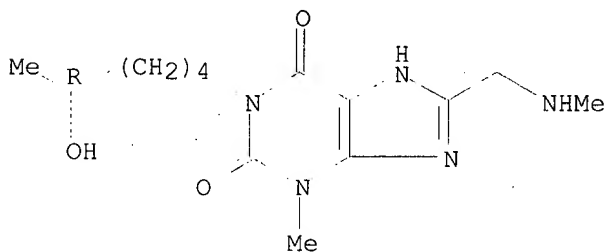
Absolute stereochemistry.



RN 301536-56-1 HCAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl-8-[(methylamino)methyl]- (9CI) (CA INDEX NAME)

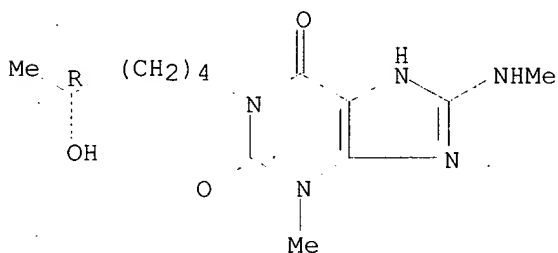
Absolute stereochemistry.



RN 301536-57-2 HCAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl-8-(methylamino)- (9CI) (CA INDEX NAME)

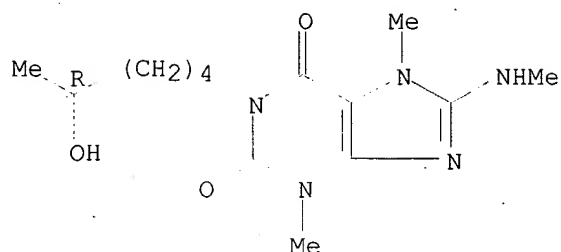
Absolute stereochemistry.



RN 301536-64-1 HCAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3,7-dimethyl-8-(methylamino)- (9CI) (CA INDEX NAME)

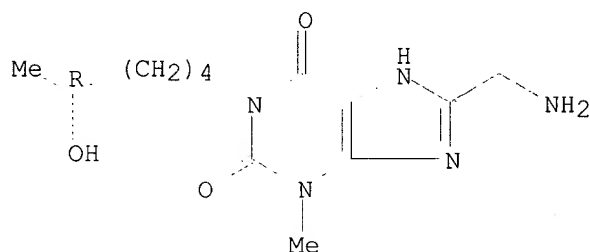
Absolute stereochemistry.



RN 403477-24-7 HCAPLUS

CN 1H-Purine-2,6-dione, 8-(aminomethyl)-3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

IT 301329-00-0P 301329-01-1P

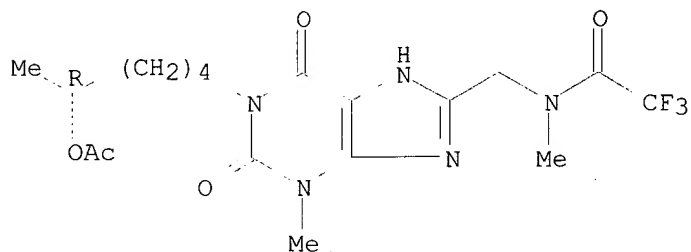
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of xanthine derivs. and analogs as cell signaling inhibitors)

RN 301329-00-0 HCAPLUS

CN Acetamide, N-[[1-[(5R)-5-(acetyloxy)hexyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl]methyl]-2,2,2-trifluoro-N-methyl- (9CI) (CA INDEX NAME)

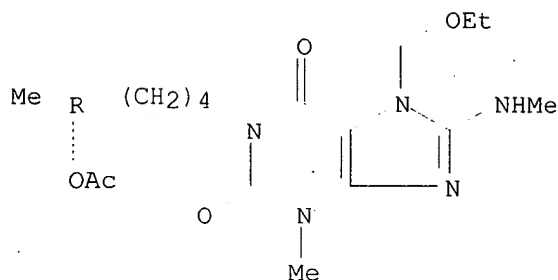
Absolute stereochemistry.



RN 301329-01-1 HCAPLUS

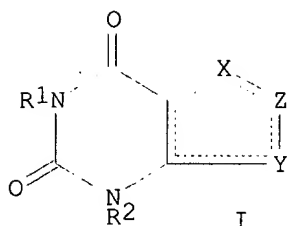
CN 1H-Purine-2,6-dione, 1-[(5R)-5-(acetyloxy)hexyl]-7-(ethoxymethyl)-3,7-dihydro-3-methyl-8-(methylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



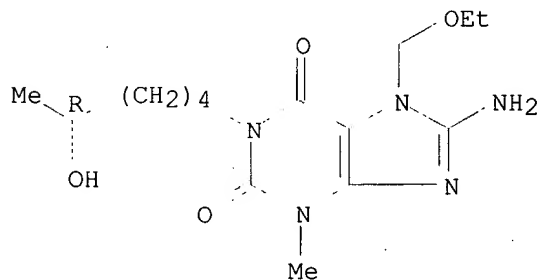
L23 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2000:742096 HCAPLUS
 DOCUMENT NUMBER: 133:296325
 TITLE: Preparation of xanthine derivatives and analogs as cell signaling inhibitors
 INVENTOR(S): Klein, J. Peter; Klaus, Stephen J.; Kumar, Anil M.; Gong, Baoqing
 PATENT ASSIGNEE(S): Cell Therapeutics, Inc., USA
 SOURCE: PCT Int. Appl., 146 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 8
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000061583	A1	2000-10-19	WO 2000-US9139	20000407
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6100271	A	20000808	US 1995-483871	19950607
US 6103730	A	20000815	US 1995-486264	19950607
US 2002028823	A1	20020307	US 1999-288556	19990409
EP 1171442	A1	20020116	EP 2000-921774	20000407
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002541258	T2	20021203	JP 2000-610854	20000407
PRIORITY APPLN. INFO.:				
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			US 1995-486264	A2 19950607
			US 1999-288556	A2 19990409
			US 1994-199368	B2 19940218
			US 1994-217051	B1 19940324
			US 1998-8020	B2 19980116
			WO 2000-US9139	W 20000407
OTHER SOURCE(S): MARPAT 133:296325				
GI				



- AB Therapeutic compds. I [R1 = H, Me, (un)substituted C5-9-alkyl, C5-9-alkenyl, C5-9-alkynyl, C3-8-hydroxyalkyl, C3-8-alkoxy, C5-9-alkoxyalkyl; R2, R3 = H, halo, oxo, (un)substituted C1-20-alkyl, C1-20-hydroxyalkyl, C(1-20)thioalkyl, C1-20-alkylamino, C1-20-alkylaminoalkyl, C1-20-aminoalkyl, C1-20-aminoalkoxyalkenyl, C1-20-aminoalkoxyalkynyl, C1-20-diaminoalkyl, C1-20-triaminoalkyl, C1-20-tetraaminoalkyl, C5-15-aminotrialkoxyamino, C1-20-alkylamido, C1-20-alkylamidoalkyl, C1-20-amidoalkyl, C1-20-acetamidoalkyl, C1-20-alkenyl, C1-20-alkynyl, C3-8-alkoxyl, C1-11-alkoxyalkyl, and C1-20-dialkoxyalkyl; with the proviso that R1 noteq. .omega.-1 secondary alc. substituted C5-8-alkyl; X, Y = NR3, R3 = C1-3-alkyl; Z = CR3, R3 = C1-3-alkyl; dashed lines are single or double bonds] pharmaceutically acceptable derivs. (e.g., resolved enantiomers, diastereomers, tautomers, salts and solvates thereof) or prodrugs thereof are described. Thus, CT11495 [I; R1 = Me R2 = (CH₂)₄CH(OH)Me-(R), X = NMe, YZ= N:CH] was prepd., via N-alkylation of 1,7-dimethylxanthine (I; R1 = Me R2 = H, X = NMe, YZ= N:CH) with (R)-5-acetoxy-1-bromohexane followed by O-deacetylation. These novel heterocyclic compds. I having a six membered ring structure fused to a five membered ring structure are found to be useful for the treatment and prevention of symptoms or manifestations assocd. with disorders affected by Interleukin-12 ("IL-12") intracellular signalling, such as, for example, Th1 cell-mediated disorders.
- IT **301328-80-3DP**, libraries
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepn. of xanthine derivs. and analogs as cell signaling inhibitors)
- RN 301328-80-3 HCAPLUS
- CN 1H-Purine-2,6-dione, 8-amino-7-(ethoxymethyl)-3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



- IT **301328-81-4DP**, 8-Amino-1-[(R)-5-Hydroxyhexyl]-3-methylxanthine,

libraries 301536-55-0P, CT 12440 301536-56-1P, CT 12441 301536-57-2P, CT 12447 301536-64-1P, CT 12481

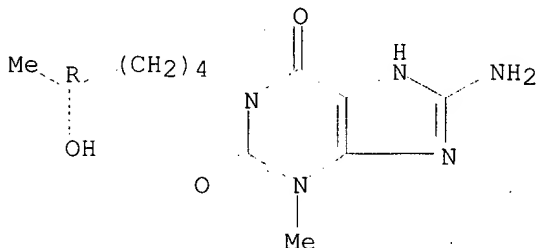
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of xanthine derivs. and analogs as cell signaling inhibitors)

RN 301328-81-4 HCAPLUS

CN 1H-Purine-2,6-dione, 8-amino-3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl- (9CI) (CA INDEX NAME)

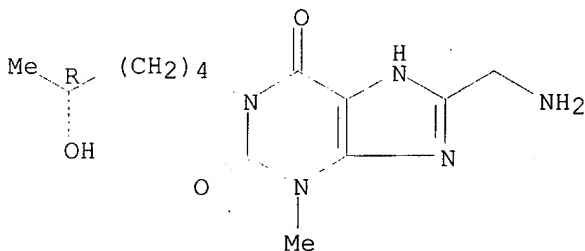
Absolute stereochemistry.



RN 301536-55-0 HCAPLUS

CN 1H-Purine-2,6-dione, 8-(aminomethyl)-3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl- (9CI) (CA INDEX NAME)

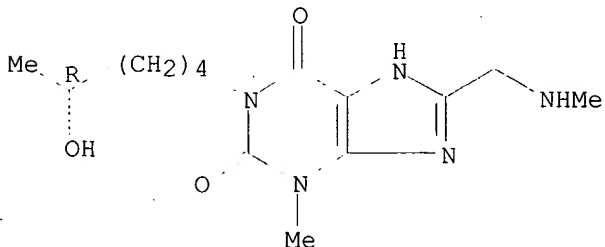
Absolute stereochemistry.



RN 301536-56-1 HCAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl-8-[(methylamino)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

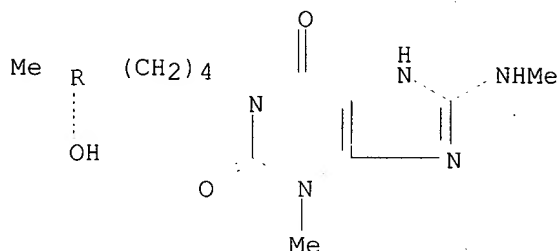


RN 301536-57-2 HCAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3-methyl-8-

(methylamino)- (9CI) (CA INDEX NAME)

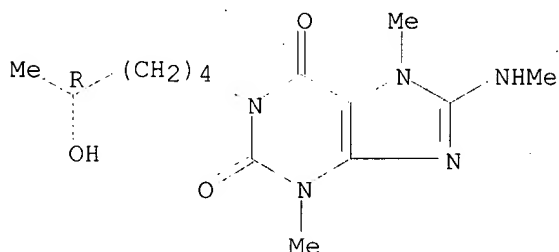
Absolute stereochemistry.



RN 301536-64-1 HCAPLUS

CN 1H-Purine-2,6-dione, 3,7-dihydro-1-[(5R)-5-hydroxyhexyl]-3,7-dimethyl-8-(methylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 301329-00-0P 301329-01-1P 301329-37-3P
301329-38-4P

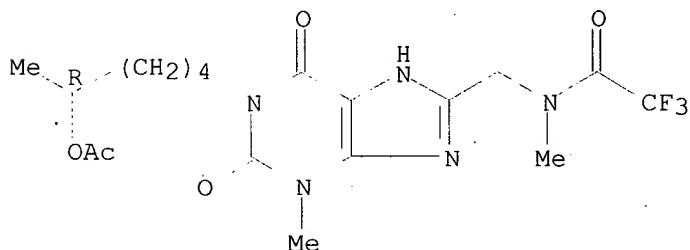
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of xanthine derivs. and analogs as cell signaling inhibitors)

RN 301329-00-0 HCAPLUS

CN Acetamide, N-[[1-[(5R)-5-(acetyloxy)hexyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl)methyl]-2,2,2-trifluoro-N-methyl- (9CI) (CA INDEX NAME)

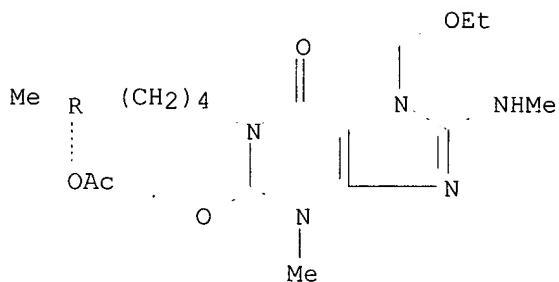
Absolute stereochemistry.



RN 301329-01-1 HCAPLUS

CN 1H-Purine-2,6-dione, 1-[(5R)-5-(acetyloxy)hexyl]-7-(ethoxymethyl)-3,7-dihydro-3-methyl-8-(methylamino)- (9CI) (CA INDEX NAME)

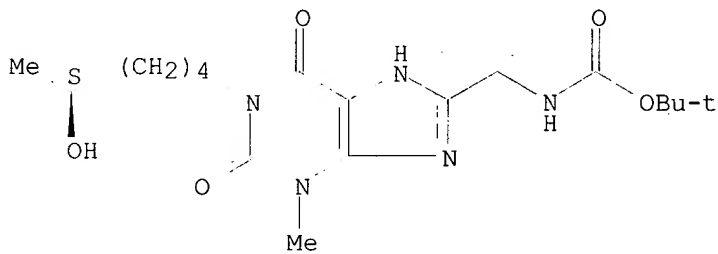
Absolute stereochemistry.



RN 301329-37-3 HCAPLUS

CN Carbamic acid, [[2,3,6,7-tetrahydro-1-[(5S)-5-hydroxyhexyl]-3-methyl-2,6-dioxo-1H-purin-8-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

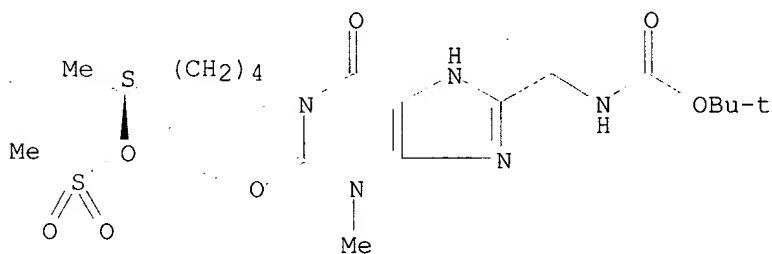
Absolute stereochemistry.



RN 301329-38-4 HCAPLUS

CN Carbamic acid, [[2,3,6,7-tetrahydro-3-methyl-1-[(5S)-5-[(methylsulfonyl)oxy]hexyl]-2,6-dioxo-1H-purin-8-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT